Master Thesis

Multi Phase Modelling an Finite Element Implementation of Steel Heat Treatment

conducted at

Institute of Mechanics,

Department of Mechanical Engineering,

TU Dortmund

by

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on

January 8, 2023

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Contents

Chapter 1

Introduction

Heat treatment of metals as a way of altering it's properties and microstructure is a process known for millennia. For many millennia heat treatment of metals has been an important part of industrial development. The ancient egypts used annealing to

The heat treatment process of steel usually involves vigorously heating the metal and throwing it into cold water. A later less vigorous reheating is optional. *Maybe spare this for the presentation*

Define feat treatment

talk about history islamic, egypt, india, china, 9000 years bc

Chapter 2

Model/Theoretical Framework/Method

Heat treatment problems require the solution of three problems. Heat transfer, mechanical material response and phase transformation are coupled by their physical interactions.

2.1 Phase Transformations

Within this work two different kind of phase transformations are treated. Martensite transformation is athermal without thermal activation while the trnsformation into bainite is diffusion controlled. The bainite transformation is time dependent while martensite transformation is only driven by cooling, c.f. Totten [2007].

For the microstructural problem two different widely accepted (sources!!!) phenomenological models are used.
The martensitic transformation relies on the Koistinen-Marburger model established by Koistinen and Marburger [1959]. It describes the transformtion using the following equation

——————————————————————— As dargelegt in the previous chapter athermal and diffusion-controlled phase transformations are treated in this thesis. The modelling of the athermal martensitic transformation relies on the Koistinen-Marburger model established in Koistinen and Marburger [1959]. It describes the transformtion using the following equation

$$\beta_M = 1 - e^{-k\,(M_S - T)} \quad .$$

$$(2.1)$$

The parameters k is material specific and describes the speed of the transformation. The martensite starting temperature M_S depends on the material and the other factors as the local carbon content that can be influenced by other phase transformations **??**.. It determines the temperature at which the transformation starts. The martensite finish temperature M_F is merely a function of the other given parameters. It is defined as the temperature at which the volume fraction of martensite reaches 0.99%.

Since the development of martensite is driven purely by cooling there is no time depen-
dence. If there is no further cooling the transformation stops. *This kind of transforma-
tion is called athermal because there is no thermal activation, no waiting time, opposite
of isothermal. In this thesis regarded as athermal also there might be something with
thermal activation going on*

Eq. 2.1 yields the development depicted in fig. 2.1 The rate of the martensitic transfor-
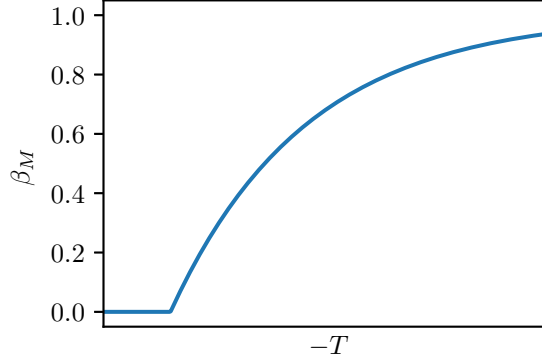

Figure 2.1: Development of the martensite volume fraction under cooling.

mation can be described by

$$\dot{\beta}_M = -e^{-k[M_S - T]}\, k\, \dot{T} = \left[1 - e^{-k[M_S - T]} - 1\right] k\, \dot{T} = -\left[1 - \beta_M\right] k\, \dot{T} \quad . \tag{2.2}$$

While this equation is valid when only considering the transformation from austenite
to martensite it can be generalized for the usage with more phase transformations by
interpreting the term $1 - \beta_M$ as the remaining austenite β_A available for transformation.
This yields the following rate for the evolution of the martensitic phase:

$$\dot{\beta}_M = -\beta_A\, k\, \dot{T} \quad . \tag{2.3}$$

The other transformations considered in this thesis are regarded as diffusion-controlled
with thermal activation. There is a time-dependence in these transformations and they
do continue isothermally when the cooling is stopped.

The equation used to describe this transformation
is the JMAK law developed by Johnson, Mehl, Avrami and Kolmogorov (Avrami,
1940; Cahn, 1956). The JMAK law

$$\beta_B = \hat{\beta}_B^{max}\left[1 - e^{-b_B\, (t^{N_B})}\right] \tag{2.4}$$

yields the sigmoidal shape seen in fig. 2.2 with a slow start and a slow finish of the
transformation but a high rate in between. It is only valid for isothermal transformations.
The parameters

$$N_B(T) = \frac{6.1273}{\ln\left(\frac{t_B^f}{t_B^s}\right)} \quad \text{and} \quad b_B(T) = \frac{0.01005}{(t_B^s)^{N_B(T)}} \tag{2.5}$$

are derived using the starting and finishing time t_B^s and t_B^f for the diffusive transfor-
mation. Those are defined at volume fraction of 1% and 99% of the target phase. The

parameters are temperature dependent and can be determined from experimental TTT diagrams (Diss Yu 1977 oder so).

The time derivation of the JMAK law eq. 2.4 yields the rate equation for isothermal cooling

$$\dot{\beta}_B = \hat{\beta}_B^{max} \, b_B \, N_B \, t^{(N_B-1)} \left[1 - \beta_B\right] \quad . \tag{2.6}$$

As the JMAK law is only valid for isothermal transformations it has to be adapted to depict a cooling process.

Something with isokinetic and additivity Scheil and Cahn.

The cooling curve is discretized into small isothermal steps at declining temperatures. Every step i is defined by it's temperature T_i and it's duration Δt_i.

In the following the procedure is explained using two isothermal steps of $\Delta t = 1.5s$ at the temperatures $T1 = 600°C$ and $T2 = 550°C$.

The first step starts at P0 with a volume fraction of bainite $\beta_B = 0$ and ends at P1 after Δt at $\beta_B^1 = 0.17$ following the transformation curve for T1. For the next step at T2, a fictitious point P1* is introduced. It is the intersection of $\beta_B = \beta_B^1$ with the transformation curve for T2. The time will be called ficitious time t^*. It is the time transformation at T2 would take to yield β_B^1.

Then transformation is again following the curve for $T2$ for a Δt of 1.5s finishing at a volume fraction β_B of 0.78.
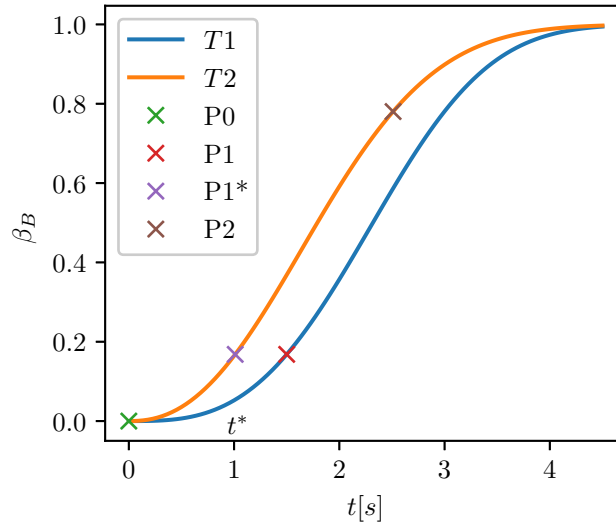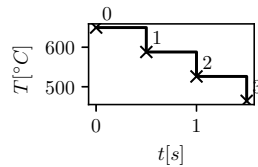

Figure 2.2: Two isothermal cooling steps.

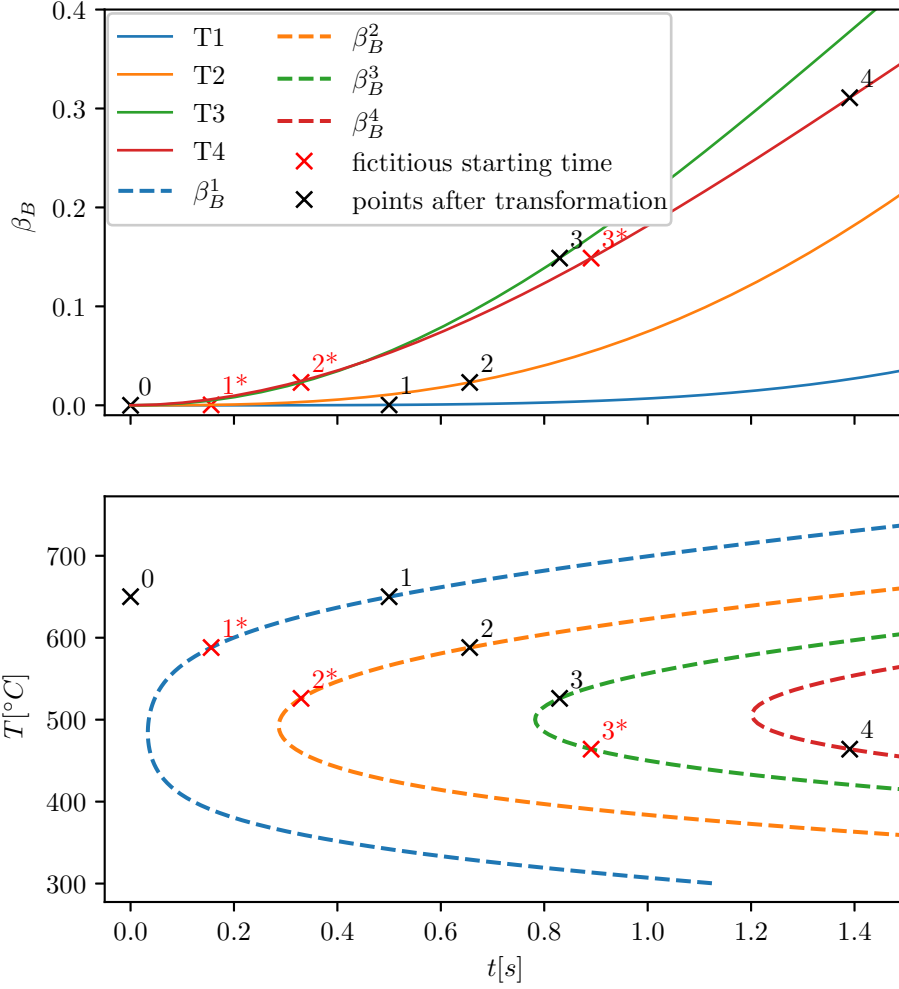Figure 2.3: Discretized example cooling curve.

Figure 2.4:

To incorporate the fictitious time into the rate equation the steps laid out in (Reti 2001) are done. Using the JMAK law 2.4, the fictitious time for a given volume fraction β_B and a temperature T the fictitious time t^* is derived as

$$t^* = \left(\frac{\ln A}{b(T_{i+1})} \right)^{\frac{1}{N(T_{i+1})}}, \quad A = \frac{\hat{\beta}}{\hat{\beta} - \beta_i} \quad . \tag{2.7}$$

This relation then is inserted into the rate equation 2.6 to replace the isothermal transformation time and eliminate the explicit time dependence

$$\dot{\beta} = N \, b^{\frac{1}{N}} \, (\hat{\beta} - \beta) \, (\ln A)^{1 - \frac{1}{N}} \quad . \tag{2.8}$$

The generalization of the rate equation for more phases *works similar* to the generalizatssion of the martensitic rate. The maximal volume fraction of bainite $\hat{\beta}$ in (Oliviera 2010) is interpreted as

$$\hat{\beta} = \beta_A = 1 - \beta_M \quad . \tag{2.9}$$

This leads to a desired coupling of the rate equations of Bainite and Martensite.

2.1.1 Involved Phases

Floris Osmond named Martensite after Adolf Martens in Osmond [1904]

2.1.2 phenomenological models

Kostinen Marburg

JMAK

Bringe ich die Metallurgie in dieses Kapitel und mische sie mit den Gleichungen oder trenne ich es in zwei Kapitel?

2.2 Thermal Problem

The thermal problem is governed by the heat equation

Chapter 3

Algorithmic implementation

After establishing the rate equations for the phase transformations 2.8 and 2.3 in the previous chapter 2 there are modifications and regularisations necessary before one is able to use them for computation. For both equations a term ζ is introduced that controls whether transformation is happening or not, cf. Pacheco et al. [2001] and de Oliveira et al. [2010].

For the martensitic transformation $\zeta_{A \to B}$ contains two heaviside functions Γ and a regularized step function using a tanh. The first heaviside function $\Gamma(-\Delta T)$ ensures irreversibility and that transformation only occurs during cooling. The second heaviside function $\Gamma(T - M_F)$ prevents transformation below the martensite finish temperature. The regularized step function $\tanh(A(M_S - T))/2 + 1/2$ starts the transformation after the temperature is blow the martensite starting temperature. The regularization deals with the discontinuity of the transformation rate at $T = M_S$. The influence of A is depicted in fig. 3.1. The choice of $A = 1$ makes the effect of the regularization disappear
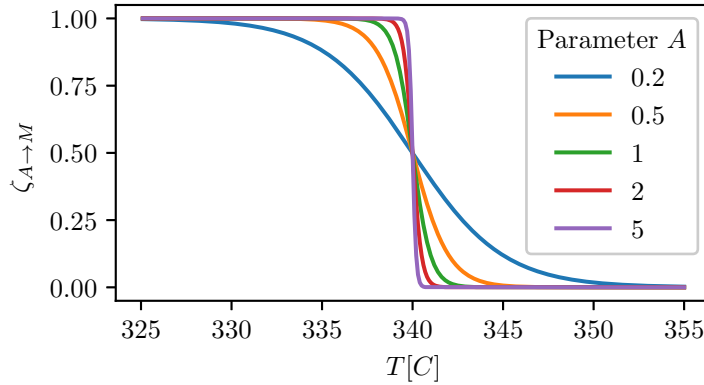

Figure 3.1: Regularized step function using a tanh with different parameters.

$(< 1e - 6)$ at $M_S \pm 2\%$.

This yields the extended rate equation for the evolution of the martensitic volume fraction

$$\dot{\beta}_M = -\zeta_{A \to M} \, \beta_A \, k \, \dot{T} \tag{3.1}$$

$$\text{with } \zeta_{A \to M} = \Gamma(-\Delta T) \, \Gamma(T - M_F) \, (\tanh(A(M_S - T))/2 + 1/2) \quad . \tag{3.2}$$

For the bainite transformation a new local time scale for every material point is

introduced. The transformation time τ starts once the temperature at the material point drops below the bainite starting temperature T_B^s. This time scale is used to account for vastly different incubation times at different temperatures. The incubation time is regarded as the time on the left of the bainite starting time t_B^s when looking at the TTT Diagram in fig. **??**..

The time on the left of the bainite starting time t_B^s when looking at the TTT Diagram in fig. **??**.. is regarded as incubation time. The incubation time τ necessary to start the transformation is vastly different at different temperatures. To account for this in a similar way to the anisothermal evolution of bainite, Scheill's additivity **?**.. is used to determine when t_B^s is reached following a cooling curve.

The following condition is checked at every time step after an update of τ to determine the start of the transformation

$$\tau = \tau + \frac{\Delta T}{t_B^s} \tag{3.3}$$

$$t_B^s \geq \tau \quad . \tag{3.4}$$

The initial value problem represented by the rate equations is solved by implicit time integration which leads to the evolution equation $\beta^{n+1} = \beta^n + \Delta\beta^{n+1}$, with $\Delta\beta^{n+1} = \Delta t \, \dot\beta^{n+1}$.

After bringing these equations into residual form

$$\underline{\mathbf{R}_{\boldsymbol\beta}} = \underline{\boldsymbol\beta}^{n+1} - \underline{\boldsymbol\beta}^n - \underline{\mathbf{\Delta}\boldsymbol\beta}$$
$$= \begin{bmatrix} R_{\beta_B} \\ R_{\beta_M} \end{bmatrix} = \begin{bmatrix} \beta_B^{n+1} - \beta_B^n - \Delta\beta_B^{n+1} \\ \beta_M^{n+1} - \beta_M^n - \Delta\beta_M^{n+1} \end{bmatrix} \tag{3.5}$$
$$\text{with } \underline{\mathbf{\Delta}\boldsymbol\beta} = f(\underline{\boldsymbol\beta}^{n+1}) \tag{3.6}$$

the backward Newton method is used to solve the equation system 3.5. The update of the backward Newton

$$\underline{\boldsymbol\beta}^{k+1} = \underline{\boldsymbol\beta}^k - \frac{\underline{\mathbf{R}_{\boldsymbol\beta}}}{\underline{\mathbf{R}_{\boldsymbol\beta'}}} \tag{3.7}$$

with the iteration counter k requires the derivation of the tangent

$$\underline{\mathbf{R}_{\boldsymbol\beta'}} = \begin{bmatrix} \frac{\partial R_{\beta_B}}{\partial \beta_B} & \frac{\partial R_{\beta_B}}{\partial \beta_M} \\ \frac{\partial R_{\beta_M}}{\partial \beta_B} & \frac{\partial R_{\beta_M}}{\partial \beta_M} \text{ with} \end{bmatrix} \tag{3.8}$$

$$\frac{\partial R_{\beta_B}}{\partial \beta_B} = 1 - \Delta t \, b^{\frac{1}{N}} \, N \left[B^{1-\frac{1}{N}} - \left(1 - \frac{1}{N}\right) B^{-\frac{1}{N}} \right] \tag{3.9}$$

$$\frac{\partial R_{\beta_B}}{\partial \beta_M} = -\Delta t \, b^{\frac{1}{N}} \, N \left[B^{1-\frac{1}{N}} - \left(1 - \frac{1}{N}\right) B^{-\frac{1}{N}} \left(1 - \frac{\beta_A}{1 - \beta_M}\right) \right] \tag{3.10}$$

$$\frac{\partial R_{\beta_M}}{\partial \beta_B} = -k \, \Delta T \, \zeta_{A \to M} \tag{3.11}$$

$$\frac{\partial R_{\beta_M}}{\partial \beta_M} = 1 - k \, \Delta T \, \zeta_{A \to M} \quad . \tag{3.12}$$

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